Applicant: Karpusas, et al. Application No.: 09/826,716

Page 2 of 9

Docket No. A062US Filed: April 5, 2001

In the Claims:

- 1.-19. (cancelled)
- 20. (currently amended) A method comprising evaluating the ability of a chemical entity to associate with an I-domain of the $\alpha 1$ chain of the $\alpha 1\beta 1$ integrin, or a complex comprising an $\alpha 1\beta 1$ integrin $\alpha 1$ -I domain, or homologs thereof, wherein:
- (a) crystallographic coordinates of the $\alpha 1\beta 1$ integrin $\alpha 1$ -I-domain of the $\alpha 1$ -chain of the $\alpha 1\beta 1$ integrin, or a complex comprising an $\alpha 1\beta 1$ integrin $\alpha 1$ -I-domain, or homologs thereof, are employed computationally or experimentally to perform used in a fitting operation between the chemical entity and said $\alpha 1\beta 1$ integrin I-domain or complex thereof, thereby obtaining data related to said association; and
- (b) the data obtained in step (a) is analyzed to evaluate the <u>degree of</u> association between the chemical entity and an I-domain of the α 1 chain of the α 1 β 1 integrin α 1-I domain, or a complex comprising an α 1 β 1 integrin α 1-I domain, or homologs thereof is evaluated in a competition assay.
- 21.-33. (cancelled).
- 34. (new) A method for evaluating the binding of a composition to an $\alpha 1\beta 1$ integrin $\alpha 1$ -I domain comprising:
- (a) crystallizing an $\alpha 1\beta 1$ integrin $\alpha 1$ -I domain by reacting a proteolytically digested $\alpha 1$ -I domain in a buffered crystallization solvent comprising a surfactant;
- (b) determining the crystal coordinates of the crystallized $\alpha 1$ -I domain;
- (c) using the crystal coordinates of the crystallized $\alpha 1$ -I domain to identify computationally a composition which bind to the $\alpha 1$ -I domain; and
- (d) using a competition assay to assess the extent to which the composition binds to the α 1-I domain.
- 35. (new) The method of claim 34, wherein the crystallization solvent comprises a PEG surfactant and a sodium-containing buffer and the crystallized α 1-I domain is frozen before its crystal coordinates are determined.
- 36. (new) The method of claim 34, wherein the proteolytically digested α 1-I domain is in a des 1-18 form.

Applicant: Karpusas, *et al*. Application No.: 09/826,716

Page 3 of 9

Docket No. A062US Filed: April 5, 2001

37. (new) The method of claim 35, wherein the proteolytically digested $\alpha 1$ -I domain is in a des 1-18 form.